Supplements

Rapid screening of very long-chain fatty acids from microorganisms

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Table 1S. Survey of literature data on the separation of fatty acids by GC. References not listed in the main article text are given below.

Column	**Stat. phase**	**Temperature program**	**tR (min)**	**tR (min)**	**Detection**	**Sample**	**References**
Omegawax 250	30 m x 0.25 mm i.d., 0.25 μm	180-270 °C (5 min) at 3 °C /min	22:6 tR = 25		FID	FAMEs from cod liver oil	[1]
Omegawax 250	15 m x 0.1 mm i.d., 0.1 μm	180-270 °C at 40 °C /min	22:6 tR = 2.03		FID	FAMEs from cod liver oil	[1]
Supercolwax 10	60 m x 0.25 mm, 0.25 μm	100 °C (1 min) - 230 °C over 7 min, 230 °C- 280 °C (10 min) over 25 min	22:6 tR = ~ 29.2	28:8 tR = ~ 32.7	GC-MS	crustacea of the order Bathynellacea	[2]
Ultra-1 capillary	25 m x 0.25 mm x 0.1 μm	50 °C (5 min) - 320 °C (15 min) at 10 °C /min			GC-MS	cyanobacterial mat of *Calothrix* sp.	[3]
Supercolwax 10	60 m x 0.25 mm, 0.25 μm	100-320 °C at 4 °C /min			GC-MS	dinoflagellates	[4]
SP™-2380	60 m x 0.25 mm, 0.2 μm	150 °C (1 min) - 180 °C at 20 °C/min, 180 °C- 250 °C (1 min) at 2 °C/min	15-24:1 tR = 38.73	21-30:1 tR = 50.29	GC-MS	*Saccharomyces pastorianus*	[5]
SE - 54	15 m x 0.32 mm	70-280 °C at 3 °C /min			FID	meibomian lipids of the mouse	[6]

Table 2S. Survey of literature data on the separation of fatty acids by HPLC. References not listed in the main article text are given below.

Column	**Stat. phase**	**Mobil. phase**	**tR (min)**	**tR (min)**	**Detection**	**Sample**	**References**
C18	75 x 4.6, 3 μm	gradient water to acetonitrile	22:6 tR = 14.5	28:8 tR = 21.3	MS2	sea anemone+ dinoflagellate	[7]
UPLC C18	150 mm x 2.1 mm, 1.7 μm	water to acetonitrile-2-propanol + aqueous ammonium acetate	22:6 tR = 6.5	28:1 tR= 49.2	positive ESI-MS, MS2	human plasma, porcine brain	[8]
C18	50 mm x 2.0 mm i.d., 3 μm	linear gradient water with 0.1% ammonium acetate and methanol with 0.1% ammonium acetate	22:6 tR = 4.76	28:1 tR = 6.91	LC-FTMS	human meibum	[9]
C18	250 mm x 4.6 mm i.d., 5 μm	isocratic acetonitrile-water (97.5:2.5, v/v)	22:6 tR = ~ 6	28:8 tR = ~ 11	evaporative light-scattering detector	dinoflagellate	[10]
preparative LC C18	300 mm x 22 mm, 10 μm	gradient acetonitrile-$CHCl_3$	22:6 tR =15	28:8 tR = 18	evaporative light-scattering detector	dinoflagellate	[10]
C8	2.1 x 50 mm, 1.7 μm	water-acetonitrile + 1 mM ammonium acetate	22:6 tR = 4.5	28:1 tR = 9.7	negative ESI-MS	fibroblasts and plasma with peroxisomal diseases	[11]
Supelcosil LC-C18	250 x 2.1 mm, 3 μm	acetonitrile + dichloromethane + propionitrile	22:6 tR = ~ 20	28:7 tR = 22.8	LC-MS with APCI	crustacea of the order Bathynellacea	[12]
C8	150 mm x 4.6 mm, 5 μm	methanol + water	22:0 tR = ~39	24:0 tR = ~47	HPLC-FD	ancient pottery	[13]
HIRPB-250AM	250 mm x 2.1 mm, 5 μm	acetonitrile + dichloromethane + propionitrile	30:1 tR = 31.5	34:1 tR =37.2	LC-MS with APCI	*Chlorella kessleri*	[14]
C8	150 mm x 3.9 mm, 5 μm	methanol + water	22:0 tR = ~8	26:0 tR = ~15	HPLC-FD	VLCFA spiked in plasma	[15]

C18	150 mm x 4.6 mm, 5 μm	methanol or methanol+2-propanol	22:0 tR = ~10	28:0 tR = ~21	LC-MS with API	standards	[16]
Zorbax ODS and C8	5-6 μm, 25 cm x 0.46 cm and 15 cm x 0.46 cm or 25 cm x 0.46 cm	acetonitrile + aqueous phosphoric acid	22:6 tR = ~ 22	18:0 tR = ~80	UV at 205 nm	bovine brain lipids	[17]
C18	100 x 8 mm, 10 μm	p-dioxane in acetonitrile	26:0 tR = ~26	26:1 tR = ~23	radioactivity flow detector	*Mycobacterium tuberculosis* H37Ra	[18]
HIRPB-250AM	250 mm x 2.1 mm, 5 μm	acetonitrile + dichloromethane + propionitrile	36:0 tR = ~40	49:0 tR = ~60	LC–MS/APCI	sugar cane wax	[19]
HIRPB-250AM	250 mm x 2.1 mm, 5 μm	acetonitrile + dichloromethane + propionitrile	22:0 tR = ~ 26	28:1 tR = ~ 31	LC–MS/APCI	*Ximenia* oil	[20]
HIRPB-250AM	250 mm x 2.1 mm, 5 μm	acetonitrile + dichloromethane + propionitrile	22:6 tR = ~ 22	22:8 tR = ~ 26	LC-MS with APCI	*Amphidinium carterae*	[21]
HIRPB-250AM	250 mm x 2.1 mm, 5 μm	acetonitrile + dichloromethane + propionitrile	23:6 tR = ~ 17	29:6 tR = ~ 37	LC-MS with APCI	*Amphidinium carterae*	[22]
C18	50 mm x 2.1 mm, 1.7 μm	acetonitrile with pentadecafluorooctanoic acid	20:0 tR = 2.0	20:6 tR = 3.3	LC-MS/MS	VLCFA in plasma	[23]

Table 3S. Commonly occurring product ions for 23:0/23:0/23:0-TAG.

m/z	Ion Description
1119.0988	Precursor ion $[M+NH_4]^+$
1102.0723	Precursor ion $[M+H]^+$
1084.0617	Precursor ion $[M+H]^+$ with loss of H_2O
747.7225	Neutral loss of sn1/sn2/sn3 $RCOOH+NH_3$ from $[M+NH_4]^+$
411.3833	sn1/sn2/sn3 acyl chain ($[RC=O+74]^+$)
393.3727	sn1/sn2/sn3 acyl chain ($[RC=O+74]^+$ with loss of H_2O)
337.3465	sn1/sn2/sn3 acyl chain ($[RC=O]^+$)
319.3359	sn1/sn2/sn3 acyl chain ($[RC=O]^+$ with loss of H_2O)

Table 4S. Commonly occurring product ions for 23:0/23:0-PC.

m/z	Ion Description
988.7951	Precursor ion $[M+acetate]^-$
914.7583	Loss of CH_3 and acetate from precursor ion
843.6848	Loss of choline and acetate from precursor ion
578.4191	Loss of sn1/sn2 acyl chain as ketene (RCH=C=O), CH_3 and acetate from precursor ion
560.4086	Neutral loss of sn1/sn2 RCOOH group, loss of CH_3 and acetate from precursor ion
353.3425	sn1/sn2 $[RCOO]^-$ ion
224.0693	Glycerophosphocholine with loss of CH_3 and H_2O
168.0431	Phosphocholine with loss of CH_3
152.9958	Glycerol-3-phosphate ion with loss of H_2O

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